Risk-Relevant Indices for the Characterization of Persistence of Chemicals in a Multimedia Environment

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OVERVIEW

- Context description: Methodologically fundamental issues in chemical hazard and risk assessment
- The central notion of overall persistence of chemicals in a multimedia environment.
- Problem formulation: Reliable quantification of persistence through appropriately defined indices
- Proposed approach – Main results
  - A new set of conceptually insightful and computationally appealing persistence indices
- Evaluation of the proposed approach in illustrative examples
- Concluding remarks
METHODOLOGICAL APPROACHES IN CHEMICAL HAZARD AND RISK ASSESSMENT

Chemical

Inherent Physicochemical Properties

Empirical

Correlations

Exposure-based indicators: Persistence, Spatial Range

Effect-based indicators: Bioaccumulation, Toxicity

- Advantages: Fast and cost-effective
- Disadvantages: Fails to capture: (i) the effect of environmental processes on the fate and distribution of chemical (ii) validity limits associated with empirically established correlations
METHODOLOGICAL APPROACHES IN CHEMICAL HAZARD AND RISK ASSESSMENT

Chemical

Inherent Physicochemical Properties → Multimedia Environmental Model + Pharmacokinetic Model

→ Concentration profiles and effective doses → Dose-Response Relationships → Risk

↑ Epidemiological Data ↑ Toxicological Data

- Advantages: Insightful, detailed, predictive
- Disadvantages: (i) Complexity
  (ii) Availability of reliable solid data
  (iii) Uncertainty
A NEW METHODOLOGICAL APPROACH (SHERINGER, 2002)

Chemical

Inherent Physicochemical Properties

+ Environmental Processes

Multimedia Environmental Model

Exposure-based indicators: Persistence, Spatial Range

Effect-based indicators: Bioaccumulation, Toxicity

- New approach represents a methodological compromise between the two previous ones – Balances realism, insightfulness with computational and practical appeal

- The multimedia environmental model is:
  (i) an evaluative one that ensures appropriate standardization when a large number of chemicals need to be screened and prioritized
  (ii) not a predictive one, i.e. is not used to determine actual concentration profiles
A NEW METHODOLOGICAL APPROACH (SHERINGER, 2002)

- Methodological advantages

(i) Introduces the requisite decoupling in a tiered framework for chemical risk assessment, i.e. can be readily used on a first-level to identify chemicals of low risk as well as chemicals of high concern that need to be further evaluated on a second-level

(ii) It is compatible with the precautionary principle and the principles of green chemistry

(iii) It is compatible with scientific criteria and methodological practices of all major regulatory frameworks for the management of chemical risk (OECD, UNEP, EU/REACH)
THE CENTRAL NOTION OF CHEMICAL PERSISTENCE

- Persistence: Temporal extent of the presence of a chemical substance in the environment (typically comprised of multiple media/phases such as soil, water and air) after its natural, accidental or intentional release

- Persistence is the most significant exposure-based risk indicator and represents a necessary condition for potentially adverse health and ecological effects

- Persistence is strongly correlated with (Scheringer, 2002):
  (i) Intake fraction (the amount that enters the human body)
  (ii) Effective dose received by the population of a certain region
  (iii) Spatial range and global pollution potential

- Persistence figures eminently on the list of scientific criteria and risk indicators currently used in all major regulatory initiatives for chemicals
THE PROBLEM

- Given a certain chemical and an evaluative multimedia environmental model that describes the fate and distribution of the chemical in the various media/phases (chemodynamics), introduce quantitative measures for persistence (persistence indices) that are:

  (i) conceptually insightful and physically meaningful

  (ii) computationally appealing

  (iii) compatible with the new methodological paradigm for chemical risk characterization

  (iv) compatible with methodological practices and scientific criteria mandated by all recent international regulatory frameworks for the management of chemicals
Structure of an environmental model showing exchange between two phases and associated degradation

Unsteady-state mass balance equations in well-mixed compartments

\[
\frac{dm_1}{dt} = -k_1 m_1 - L_{12} m_1 + L_{21} m_2
\]

\[
\frac{dm_2}{dt} = -k_2 m_2 - L_{21} m_2 + L_{12} m_1
\]
Prototypical Environmental Model With Three Media: Soil, Water, Air
(Unit-World Model)
- Unsteady-state mass balance equations for the three phases/media:

\[
\begin{align*}
\frac{dm_s}{dt} &= -(k_s + L_{sw} + L_{sa})m_s + L_{ws}m_w + L_{as}m_a \\
\frac{dm_w}{dt} &= L_{sw}m_s - (k_w + L_{ws} + L_{wa})m_w + L_{aw}m_a \\
\frac{dm_a}{dt} &= L_{sa}m_s + L_{wa}m_w - (k_a + L_{as} + L_{aw})m_a
\end{align*}
\]

\[
m = \begin{bmatrix} m_s \\ m_w \\ m_a \end{bmatrix} = \text{vector of masses in media (s,w,a)}
\]

\[
K = \begin{bmatrix} k_s & 0 & 0 \\ 0 & k_w & 0 \\ 0 & 0 & k_a \end{bmatrix} = \text{Matrix of degradation rate constants}
\]

\[
L = \begin{bmatrix} -(L_{sw} + L_{sa}) & L_{ws} & L_{as} \\ L_{sw} & -(L_{ws} + L_{wa}) & L_{aw} \\ L_{sa} & L_{wa} & -(L_{as} + L_{aw}) \end{bmatrix} = \text{Phase transfer coefficient matrix}
\]

Intermedia transport through diffusive and advective mass transfer (several mechanisms)
### TABLE 1: Phase Volumes and Interfacial Areas (Scheringer, 1996)

<table>
<thead>
<tr>
<th>Process Volumes and Interfacial Areas</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil Volume $V_s$</td>
<td>1 m$^3$</td>
</tr>
<tr>
<td>Water Volume $V_w$</td>
<td>233 m$^3$</td>
</tr>
<tr>
<td>Air Volume $V_a$</td>
<td>$2 \times 10^5$ m$^3$</td>
</tr>
<tr>
<td>Air/Soil interfacial area $A_{as}$</td>
<td>10</td>
</tr>
<tr>
<td>Air/Water interfacial area $A_{aw}$</td>
<td>23.3</td>
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### TABLE 2: Process Parameters (Scheringer, 1996)

<table>
<thead>
<tr>
<th>Process Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transfer velocity (water) $u_w$</td>
<td>0.72 m/day</td>
</tr>
<tr>
<td>Transfer velocity (air over water) $u_{a1}$</td>
<td>72 m/day</td>
</tr>
<tr>
<td>Transfer velocity (air over soil) $u_{a2}$</td>
<td>24 m/day</td>
</tr>
<tr>
<td>Transfer velocity (air in soil) $u_{s1}$</td>
<td>0.16 m/day</td>
</tr>
<tr>
<td>Transfer velocity (water in soil) $u_{s12}$</td>
<td>$6.2 \times 10^{-5}$ m/day</td>
</tr>
<tr>
<td>Dry deposition velocity $u^{dry}$</td>
<td>260 m/day</td>
</tr>
<tr>
<td>Wet deposition velocity $u^{wet}$</td>
<td>460 m/day</td>
</tr>
<tr>
<td>Rain rate $u^{rain}$</td>
<td>$2.3 \times 10^{-3}$ m/day</td>
</tr>
<tr>
<td>Water runoff rate $u_r^{runoff}$</td>
<td>$9.4 \times 10^{-4}$ m/day</td>
</tr>
<tr>
<td>Soil runoff rate $u_s^{runoff}$</td>
<td>$5.5 \times 10^{-7}$ m/day</td>
</tr>
<tr>
<td>Gas Constant $R$</td>
<td>8.314 Pa m$^3$/mol K</td>
</tr>
<tr>
<td>Temperature $T$</td>
<td>290 K</td>
</tr>
<tr>
<td>Fraction organic carbon $f_{oc}$</td>
<td>0.02</td>
</tr>
<tr>
<td>Vapor-particle partitioning coefficient $\Phi$</td>
<td>[0,1]</td>
</tr>
</tbody>
</table>
TABLE 3: Fugacity Capacities (Scheringer, 1996; Bennett et al., 1999)

<table>
<thead>
<tr>
<th>Medium</th>
<th>Fugacity Capacity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>$Z_{air} = \frac{1}{RT_{air}}$</td>
</tr>
<tr>
<td>Water</td>
<td>$Z_{water} = \frac{1}{K_{HI}}$</td>
</tr>
<tr>
<td>Soil</td>
<td>$Z_{soil} = 0.41 f K_{oc \cdot ow}$</td>
</tr>
</tbody>
</table>

TABLE 4: Phase Transfer Coefficients (Scheringer, 1996; Bennett et al., 1999)

<table>
<thead>
<tr>
<th>Phase Transfer Mode</th>
<th>Phase Transfer Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air to water - Diffusive</td>
<td>$L_{diff}^{aw} = \frac{u_{aw} l_{a1} l_{air}}{u_{w} + u_{a1} l_{air}} \left( \frac{Z_{water}}{V_{a}} \right)$</td>
</tr>
<tr>
<td>Water to air - Diffusive</td>
<td>$L_{diff}^{wa} = l_{aw} \frac{Z_{air}}{Z_{water}} V_{a}$</td>
</tr>
<tr>
<td>Air to soil - Diffusive</td>
<td>$L_{diff}^{as} = \left[ u_{a2} \left( \frac{Z_{water}}{Z_{air}} \right) A_{as} V_{a} \right] \left[ 1 + \left( \frac{u_{a2} l_{a1} l_{air}}{u_{a2} + u_{a1} l_{air}} \frac{Z_{water}}{Z_{air}} \right) \right]$</td>
</tr>
<tr>
<td>Soil to air - Diffusive</td>
<td>$L_{diff}^{sa} = L_{diff}^{as} \frac{Z_{air}}{Z_{soil}} V_{a}$</td>
</tr>
<tr>
<td>Air to soil – Rain washout</td>
<td>$L_{rain}^{as} = u_{rain} \frac{Z_{water}}{Z_{air}} A_{as} V_{a}$</td>
</tr>
<tr>
<td>Air to water – Rain washout</td>
<td>$L_{rain}^{aw} = u_{rain} \frac{Z_{water}}{Z_{air}} A_{aw} V_{a}$</td>
</tr>
<tr>
<td>Air to soil – Particle deposition</td>
<td>$L_{dep}^{as} = \left( u_{dry} + u_{wet} \right) A_{as} \frac{V_{a}}{v_{a}}$</td>
</tr>
<tr>
<td>Air to water – Particle deposition</td>
<td>$L_{dep}^{aw} = \left( u_{dry} + u_{wet} \right) A_{aw} \frac{V_{a}}{v_{a}}$</td>
</tr>
<tr>
<td>Soil to water</td>
<td>$L_{aw} = \left( u_{w} \frac{Z_{water}}{Z_{soil}} \right) + u_{s} \frac{runoff}{v_{s}} A_{as} \frac{V_{a}}{v_{a}}$</td>
</tr>
<tr>
<td>Air to water - Overall</td>
<td>$L_{aw} = \left( L_{diff}^{aw} + L_{rain}^{aw} \right) \left( 1 - \Phi \right) L_{dep}^{aw} \Phi$</td>
</tr>
<tr>
<td>Air to soil - Overall</td>
<td>$L_{as} = \left( L_{diff}^{aw} + L_{rain}^{aw} \right) \left( 1 - \Phi \right) L_{dep}^{as} \Phi$</td>
</tr>
<tr>
<td>Soil to air</td>
<td>$L_{sa} = 0.001 L_{dep}^{as} \Phi + L_{diff}^{sa}$</td>
</tr>
</tbody>
</table>
- Multimedia environmental model can be represented in a compact form:

\[
\frac{dm}{dt} = Am = (-K + L)m
\]

- Dynamic distribution of chemical in different media:

\[
m(t) = \begin{bmatrix} m_s(t) \\ m_w(t) \\ m_a(t) \end{bmatrix} = \exp(At)m_0
\]

where

\[
m_0 = \begin{bmatrix} m_{s,0} \\ m_{w,0} \\ m_{a,0} \end{bmatrix} = \text{vector of initial masses (release pattern/discharge conditions)}
\]

- Multimedia environmental models are very suitable for describing the behavior of non-polar organic chemicals, and most importantly Persistent Organic Pollutants (POPs; dioxins, PCBs, DDT) which are of high-concern due to their adverse health and ecological effects (UNEP 2003).
QUANTITATIVE PERSISTENCE MEASURES: EXISTING APPROACHES

- (I) Multiple half-life approach: Chemical is declared persistent if any one of its half-lives in different media exceeds a certain threshold value. Limitations: Uses only inherent physicochemical properties and overlooks intermedia transport and phase partitions, frequently leading to misclassification (focuses on half-lives in media into which the chemical seldom partitions)

- (II) Chemical clearance time: Time required for the chemical’s total concentration to drop below a pre-specified level Limitations: (i) Exact release/discharge conditions are often uncertain (ii) Could lead to underestimation of actual persistence due to low concentration levels in a medium into which partitioning is favorable and degradation quite slow

- (III) Characteristic-time at the remote/asymptotic state: Inverse of the model’s slowest eigenvalue (slowest time-scale of underlying chemodynamics that determines its asymptotic behavior) Limitations: Does not take into account the entire dynamic history of the chemical’s environmental behavior
QUANTITATIVE PERSISTENCE MEASURES: EXISTING APPROACHES

- (IV) Residence Time (also known as “equivalence width”):

\[
\tau = \frac{1}{M_0} \int_0^\infty M(t)dt = \frac{1}{(m_{s,0} + m_{w,0} + m_{a,0})} \int_0^\infty \{m_s(t) + m_w(t) + m_a(t)\}dt
\]

\[
M_0 = m_{s,0} + m_{w,0} + m_{a,0} = \text{initial total mass}
\]

\[
M(t) = m_s(t) + m_w(t) + m_a(t) = \text{total mass}
\]

If:

\[
V = \begin{bmatrix}
  v_s & 0 & 0 \\
  0 & v_w & 0 \\
  0 & 0 & v_a
\end{bmatrix}
\]

\[
e = \begin{bmatrix}
  e_1 \\
  e_2 \\
  e_3
\end{bmatrix} = -V^{-1}Am_0
\]

Then:

\[
\tau = \frac{1}{M_0}(e_1v_1 + e_2v_2 + e_3v_3)
\]

-Advantages: i) Captures entire dynamic environmental history of chemical (inherent physicochemical properties + environmental processes)
  ii) Conceptually insightful/Practically appealing

-Disadvantages: i) Dependence on release pattern and associated uncertainties
  ii) Standardization problems arise when used for chemicals classification and screening purposes
PROPOSED APPROACH: MAIN RESULTS

- Residence-time as a persistence index can be rewritten as follows:

\[
\tau = \frac{1}{M_0} \int_0^\infty M(t)dt = \frac{1}{(m_{s,0} + m_{w,0} + m_{a,0})} \int_0^\infty \{m_s(t) + m_w(t) + m_a(t)\}dt = \frac{1}{\|m_0\|_1} \int_0^\infty \|m(t)\|_1 dt
\]

where \(\|x\|_1 \equiv \sum_{i=1}^n |x_i|\) = 1-norm of vector \(x\)

- Consider an alternative index that conceptually relies on an “envelope” encompassing all possible chemodynamic trajectories and behavior induced by all possible initial conditions (release patterns):

\[
\tau_1 = \int_0^\infty \max_{m_0 \neq 0} \frac{\|m(t)\|_1}{\|m_0\|_1} dt = \int_0^\infty \max_{m_0 \neq 0} \frac{\|\exp(At)m_0\|_1}{\|m_0\|_1} dt
\]
PROPOSED APPROACH: MAIN RESULTS

- From matrix algebra it is known that:

\[
\max_{m_0 \neq 0} \frac{\|\exp(At)m_0\|_1}{\|m_0\|_1} = \|\exp(At)\|_1 = \text{1-norm of exponential matrix}
\]

\[
= \max_{1 \leq j \leq 3} \sum_{i=1}^{3} |(\exp(At))_{i,j}| = \text{maximum column sum of exponential matrix (can be easily calculated using MATLAB)}
\]

where \((\exp(At))_{i,j}\) = is the \((i,j)\)-th entry of the exponential matrix

- Therefore, the proposed persistence index takes the form:

\[
\tau_1 = \int_{0}^{\infty} \|\exp(At)\|_1 dt
\]
PROPOSED APPROACH: MAIN RESULTS

- Proposed persistence index:
  
i) relies on a multimedia environmental model that integrates inherent physicochemical properties with environmental processes

ii) captures the entire dynamic history of the chemical’s environmental behavior

iii) can be readily calculated using simple MATLAB commands

iv) does not depend on a specific release pattern and the particular discharge conditions, and therefore, effectively overcomes standardization problems at the chemicals classification and screening stage

v) introduces a measure of “conservativeness” that is aligned with the precautionary principle and the principles of green chemistry
- Consider an alternative persistence index (frequently used in the analysis and environmental management of ecological systems):

\[
\tau = \frac{2}{m_0^T m_0} \int_0^{\infty} m^T(t)m(t)dt = \frac{2}{(m_{s,0}^2 + m_{w,0}^2 + m_{a,0}^2)} \int_0^{\infty} \{m_s^2(t) + m_w^2(t) + m_a^2(t)\}dt
\]

- Introduces a measure of “distance” between the current dynamic state of the chemical’s environmental behavior and its final relaxation state, i.e. state of ultimate decay in a multimedia environment, and the associated time to “cover” it.

- One can show that the above persistence measure can be calculated analytically:

\[
\tau = \frac{2}{m_0^T m_0} (m_0^T P m_0)
\]

where matrix $P$ is the solution of the Lyapunov matrix equation (easily calculated using MATLAB):

\[
A^T P + PA = -I
\]

(A being the model’s characteristic matrix and I the identity matrix)
- In a spirit similar to the one in the previous case, the following persistence index is proposed:

\[
\tau_2 = \max_{m_0 \neq 0} \frac{2}{m_0^T m_0} (m_0^T P m_0)
\]

- Using a pertinent result of matrix theory, the above maximization yields:

\[
\tau_2 = 2 \lambda_{\text{max}}(P)
\]

where \( \lambda_{\text{max}}(P) \) is the largest eigenvalue of matrix P (it can be proven that P has only positive eigenvalues)
PROPOSED APPROACH: MAIN RESULTS

-Proposed persistence index:
  i) relies on a multimedia environmental model that integrates inherent physicochemical properties with environmental processes
  ii) captures the entire dynamic history of the chemical’s environmental behavior
  iii) can be analytically calculated
  iv) does not depend on a specific release pattern and the particular discharge conditions, and therefore, effectively overcomes standardization problems at the chemicals classification and screening stage
  v) introduces a measure of “conservativeness” that is aligned with the precautionary principle and the principles of green chemistry
  vi) Amenable to direct nonlinear generalization
PROPOSED APPROACH: MAIN RESULTS

- Upper and lower bounds on both $\tau_1, \tau_2$ can be mathematically established.
- As intuitively expected:

$$
\tau_1 \geq \frac{1}{|\lambda_{sl}|} = \tau_{1}^{LB}
$$

$\lambda_{sl}$ is the absolute value of the slowest eigenvalue of $A$ that governs the asymptotic chemodynamic behavior.

$$
\tau_2 \geq \frac{1}{|\lambda_{sl}|} = \tau_{2}^{LB}
$$

(if $-\lambda_1 < -\lambda_2 < -\lambda_3$ with $\lambda_1 > \lambda_2 > \lambda_3$

then $|\lambda_{sl}| = \lambda_3$ )

- Upper bounds can be also derived (shown in paper), however, they do not seem to carry any particular physical meaning.

-Both lower and upper bounds are practically useful in a tiered screening framework:

(i) Lower bounds could be used for the identification of persistence chemicals of high concern when large values are computed.

(ii) Upper bounds could be used for the identification of chemicals that are not persistent when numerically small values are computed.
<table>
<thead>
<tr>
<th>Chemical</th>
<th>$k_s$ ($s^{-1}$)</th>
<th>$k_w$ ($s^{-1}$)</th>
<th>$k_a$ ($s^{-1}$)</th>
<th>Log ($K_{ow}$)</th>
<th>$K_H$ ($Pa \ m^3 \ mol^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CCl_3F$</td>
<td>$2.93 \times 10^{-8}$</td>
<td>$2.93 \times 10^{-8}$</td>
<td>$2.72 \times 10^{-10}$</td>
<td>2.53</td>
<td>$9.83 \times 10^3$</td>
</tr>
<tr>
<td>1-butanol</td>
<td>$2 \times 10^{-6}$</td>
<td>$2 \times 10^{-6}$</td>
<td>$3.99 \times 10^{-6}$</td>
<td>0.88</td>
<td>$5.64 \times 10^{-1}$</td>
</tr>
<tr>
<td>Dioxane</td>
<td>$7.71 \times 10^{-8}$</td>
<td>$7.71 \times 10^{-8}$</td>
<td>$4.32 \times 10^{-6}$</td>
<td>-0.27</td>
<td>$4.94 \times 10^{-1}$</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>$7.71 \times 10^{-8}$</td>
<td>$7.71 \times 10^{-8}$</td>
<td>$4.03 \times 10^{-6}$</td>
<td>3.44</td>
<td>$1.95 \times 10^4$</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>$7.36 \times 10^{-8}$</td>
<td>$7.36 \times 10^{-8}$</td>
<td>$4.80 \times 10^{-7}$</td>
<td>2.84</td>
<td>$3.49 \times 10^2$</td>
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<tr>
<td>Benzene</td>
<td>$7.64 \times 10^{-7}$</td>
<td>$7.64 \times 10^{-7}$</td>
<td>$6.99 \times 10^{-7}$</td>
<td>2.13</td>
<td>$5.50 \times 10^2$</td>
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<td>DDT</td>
<td>$2.50 \times 10^{-9}$</td>
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<td>5.98</td>
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<tr>
<td>Chemical</td>
<td>$\tau_1$ (days)</td>
<td>$\tau_2$ (days)</td>
<td>$\tau_{sl}$ (days)</td>
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</tr>
<tr>
<td>-----------</td>
<td>-----------------</td>
<td>-----------------</td>
<td>--------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$CCl_3F$</td>
<td>$4.13 \times 10^4$</td>
<td>$12.1 \times 10^4$</td>
<td>$4.03 \times 10^4$</td>
<td></td>
<td></td>
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<tr>
<td>1-butanol</td>
<td>7.14</td>
<td>6.7</td>
<td>5.74</td>
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<tr>
<td>Dioxane</td>
<td>124.45</td>
<td>226</td>
<td>123.94</td>
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<tr>
<td>Cyclohexane</td>
<td>15.52</td>
<td>13.28</td>
<td>12.73</td>
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<td>51.2</td>
<td>24.47</td>
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<td>29.6</td>
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<td>$4.48 \times 10^3$</td>
<td>$4.48 \times 10^3$</td>
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<td></td>
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<tr>
<td>Chemical</td>
<td>Lower Bound (days)</td>
<td>$\tau_1$ (days)</td>
<td>Upper Bound (days)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>--------------------</td>
<td>-----------------</td>
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<tr>
<td>$CCl_3F$</td>
<td>$4.03 \times 10^4$</td>
<td>$4.13 \times 10^4$</td>
<td>$12.11 \times 10^4$</td>
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<td>5.74</td>
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<td>13.28</td>
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<td>15.52</td>
<td>23.61</td>
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<td>Chlorobenzene</td>
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<td>75.03</td>
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<td>17.05</td>
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<td>$4.49 \times 10^3$</td>
<td>$7.76 \times 10^3$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
## TABLE 8: Upper and Lower Bounds of $\tau_2$

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Lower Bound (days)</th>
<th>$\tau_2$ (days)</th>
<th>Upper Bound (days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CCl_3F$</td>
<td>$4.03 \times 10^4$</td>
<td>$12.1 \times 10^4$</td>
<td>*</td>
</tr>
<tr>
<td>1-butanol</td>
<td>5.74</td>
<td>6.7</td>
<td>6.92</td>
</tr>
<tr>
<td>Dioxane</td>
<td>123.94</td>
<td>226</td>
<td>*</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>12.73</td>
<td>13.28</td>
<td>14.75</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>24.47</td>
<td>51.2</td>
<td>85.4</td>
</tr>
<tr>
<td>Benzene</td>
<td>16.55</td>
<td>29.6</td>
<td>*</td>
</tr>
<tr>
<td>DDT</td>
<td>$4.48 \times 10^3$</td>
<td>$4.48 \times 10^3$</td>
<td>$4.54 \times 10^3$</td>
</tr>
</tbody>
</table>
CONCLUSIONS

• A new set of persistence indices is proposed.

• The proposed persistence indices allow a reliable quantitative characterization of persistence of chemicals in a multimedia environment, while overcoming some of the limitations associated with existing approaches.

• On a theoretical level, they are: (i) conceptually inspired by notions of characteristic time found in systems science, and (ii) technically based on results from matrix theory

• Finally, on a practical level, the proposed persistence indices can be readily calculated using simple MATLAB commands and incorporated into the model-based scientific criteria and methodological practices associated with recently emerging international regulatory regimes for the management of chemicals
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